

**FINAL REPORT for NASA grant  
NAG3-1841:  
Project Title: Theoretical Studies of  
Liquid  $^4\text{He}$  near the Superfluid  
Transition**

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We performed theoretical studies of liquid helium by applying state of the art simulation and finite-size scaling techniques. We calculated universal scaling functions for the specific heat and superfluid density for various confining geometries relevant for experiments such as the confined helium experiment and other ground based studies. We also studied microscopically how the substrate imposes a boundary condition on the superfluid order parameter as the superfluid film grows layer by layer. Using path-integral Monte Carlo, a quantum Monte Carlo simulation method, we investigated the rich phase diagram of helium monolayer, bilayer and multilayer on a substrate such as graphite. We find excellent agreement with the experimental results using no free parameters. Finally, we carried out preliminary calculations of transport coefficients such as the thermal conductivity for bulk or confined helium systems and of their scaling properties. All our studies provide theoretical support for various experimental studies in microgravity.

## 1 Task Description

Using Monte Carlo techniques, such as cluster Monte Carlo, which eliminate the long-standing problem of critical-slowing-down, we can approach close to the lambda point for large-size lattices and, thus, extract the critical exponents and scaling properties of the physical quantities of interest. Our previous studies indicated that we can achieve very good agreement with the experimentally determined universal function for the specific heat of confined helium if appropriate boundary conditions are used. We carried out these calculations and we obtained accurate results and even better understanding of the finite-size effects in both the specific heat and superfluid density. Other finite geometries, such as the pore geometry were studied and our calculated universal functions were compared to experimental data. From the calculated universal function for the specific heat we made predictions for the confined helium experiment (CHEX) and our prediction came in close agreement with the results of CHEX.

In addition, we studied microscopically the role of the substrate in determining the boundary conditions. For the latter studies, we used path integral quantum Monte Carlo (PIMC) methods using the bare helium-helium interaction potential. The role of the substrate in determining the boundary condition on the order parameter and its derivative at the boundary is very important. Using PIMC we investigated the rich phase diagram of helium monolayer, bilayer and multilayer on graphite. We found excellent agreement with numerous phases and features revealed in various experimental studies using no free parameters in our calculations.

In addition, the finite-size scaling and critical exponents of the thermal conductivity of bulk and confined helium was studied. For this work we used dynamical models, such as the so-called model-F, using real-time evolution of an ensemble of systems at a given temperature and from that we extracted the appropriate correlation functions.

## 2 Task Significance

The space experiment CHEX was designed to test the validity of finite-size-scaling (FSS) theory of critical phenomena[1, 2, 3]. If the system is confined in geometries of reduced dimensionality, when the critical point is approached,

the correlation length can become as large as the size of the confining length. In this case the values of global properties of the system, such as specific heat, are significantly different from their values for the bulk system. FSS theory can be used to determine the general dependence of a global property on the confining length-size near the critical point.

Though earlier experiments on superfluid helium films of finite thickness [4] seemed to confirm the validity of the FSS, there were more recent experiments[5, 6] where it was shown that the superfluid density of thick helium films does not satisfy FSS when the expected values of critical exponents were used. Similarly, in previous measurements of the specific heat of helium in finite geometries, other than the expected values for the critical exponents were found [7].

Recently the results and the conclusions of the analysis of the experiment CHEX have been published[17] as well as those of more recent ground-based experiments[8, 9]; they are found to be in general agreement with the expectations from RG theory[10, 11, 12, 13]. Moreover, it was concluded[17] that the scaling function was in very good agreement with our prediction[18] based on numerical simulations of a model which belongs to the same universality class as the superfluid transition. In addition, the results of these simulations which were available well before the flight experiment, helped the CHEX team plan the experiment. Fig. 1 is taken from Ref.[17] where the CHEX collaboration compares their results with theoretical predictions.

Since the renormalization group calculations are approximate, numerical investigations of the finite-size scaling properties of static and dynamic critical properties need to be carried out as an independent tool to study the validity of the theory. In addition, the role of the van der Waals forces in thin films cannot be addressed by the conventional renormalization group theoretical methods.

The simulation techniques could be considered “exact” for a given finite size system; however, the limitation of this approach is the finite system size used in the simulations. To obtain control over this problem

a) we have developed and adopted algorithms such as the so-called cluster algorithm[14], the over-relaxation method[15], the Metropolis algorithm as well as combination of these updates to produce more efficient hybrids.

b) we have extended the path integral Monte Carlo method[16] to study inhomogeneous systems, such as films where the role of the substrate is important[20, 21, 22].

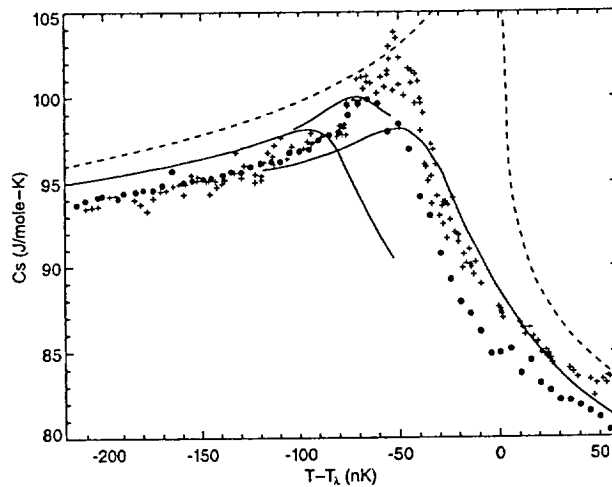


Figure 1: Comparison of the theoretical expectations to the CHeX results (Solid Circles). This figure is taken from the paper by *J. Lipa, et al.*, to appear in Phys. Rev. Lett. The plus signs are the results of simulations (Schultka and Manousakis[18]). The solid lines are results from Dohm's group. The dashed line is the result for bulk.

c) we constructed a massively parallel cluster of processors with very high performance to cost ratio which we are using to simulate critical static and dynamic properties.

Our objective was to apply all the above tools to calculate static properties of superfluid helium near the superfluid transition temperature and to carry out finite-size scaling with direct objective to make predictions for the main planned low temperature space experiments.

### 3 Progress During the Funding Period

We have used state of the art simulation techniques to study equilibrium critical properties and finite size scaling of confined helium. We have completed a comprehensive numerical study of both the superfluid density[23, 24, 25] and the specific heat[26, 27, 29, 30, 31] of the x-y model on lattices which correspond to film and pore geometries using the Cluster Monte Carlo method. We have studied the crossover from one and from two to three dimensional

superfluidity. We have computed the scaling function for the specific heat and superfluid density which depend on the geometry and on the boundary conditions applied.

We investigated the scaling of the superfluid density in superfluid films using Dirichlet boundary conditions along the direction of the film-thickness. We studied the scaling of the superfluid density with respect to the film thickness  $H$  by simulating the x-y model on films of size  $L \times L \times H (L \gg H)$  using the cluster Monte Carlo. Periodic boundary conditions were used in the planar ( $L$ ) directions and Dirichlet boundary conditions along the film thickness. We find that the system exhibits a Kosterlitz-Thouless phase transition at the  $H$ -dependent critical temperature below the critical temperature ( $\lambda$ ) of the bulk system. However, right at the critical temperature the ratio of the areal superfluid density to the critical temperature turns out to be  $H$ -dependent in the range of film thicknesses considered. We do not observe finite-size scaling of the superfluid density with respect to  $H$ . However, the numerical data obtained by our simulation techniques can be collapsed onto one universal curve by introducing an effective thickness  $H_{eff} > H$  into the corresponding scaling relations. We argued that the effective thickness depends on the type of boundary conditions.

The scaling function  $f_1$  of the specific heat is not very sensitive to this boundary effect within error bars. Our results for the specific heat scaling function obtained for Dirichlet boundary conditions along the finite dimension of the film (film thickness) has been compared with the recently analyzed results of the Confined Helium experiment (CHeX). Lipa et al.[17] find good agreement between the CHeX results and our predictions. There are also experimental results on the specific heat scaling function in the pore geometry[31] and the comparison with our results is also reasonably good.

We have built a 64-processor dedicated massively parallel cluster with a very high performance/cost ratio. Using this dedicated cluster and state of the art simulation techniques we have studied dynamical properties of confined helium. First we studied the finite-size scaling behavior of thermal resistivity near the  $\lambda$  point of helium confined in pore-like geometry[32, 33, 34] similar to the experiment BEST (Boundary Effects near the Superfluid Transition) which will be a future microgravity fundamental physics experiment with principal investigators Professor Ahlers of UCSB and Dr F-C. Liu of JPL. Our calculated thermal resistivity obeys scaling using the same dynamical exponent found by Ahlers in earlier experimental studies.

In addition, our scaling curve is in reasonable agreement with the results of Kahn and Ahlers.[35] Further investigation is required to study the role of boundary condition and geometry.

We have also studied the layer by layer growth of helium-4 on graphite, originally looking for a microscopic determination of the boundary condition on the order parameter of a confined superfluid. In that search we found that the system develops a very rich phase diagram in its layer by layer growth on graphite. To study helium-4 on graphite we have developed a direct and very powerful tool. Starting from the bare helium-helium and helium-graphite interactions we use the path integral Monte Carlo (PIMC) method where particle permutations are also sampled. To develop such an accurate method it took us several years but very interesting results have begun to emerge. First, we have examined the first adsorbed layer[20, 21, 22] and have reproduced numerous features of this layer seen in experiment. Commensurate, domain wall, and incommensurate solid structures are all reproduced by our methods. The melting behavior of the commensurate solid has been studied in detail and a melting temperature in good agreement with experiment has been determined. We also determine the single particle binding energy and the coverage at which the second layer begins to be occupied. Both are in excellent agreement with experiment. We have also examined the low density, low temperature region of the phase diagram, which is more experimentally controversial. Our calculations have been able to directly demonstrate that this region consists of a low- density vapor and solid helium clusters. We find no first layer superfluidity, as some recent experiments had suggested.

In the second adsorbed layer[20, 21], we have identified gas, superfluid liquid, commensurate-solid, and incommensurate-solid phases, and the coexistence regions between them. The phase boundaries and the specific heat are in good agreement with experiment. The appearance and disappearance of superfluidity with increasing coverage can be explained by the growth of coexistence phases, as was observed by torsional oscillator experiments. We have performed calculations of multiple layers of helium on graphite[37, 38, 39, 40]. We find that the system produces at least five atomically thin layers. The third and fourth layers possess self-bound superfluid liquid phases. We have determined the low-temperature equilibrium density of these phases, which are in good agreement with experiment. At low third layer densities, we have observed liquid-gas coexistence and a metastable liquid phase. The spinodal

point that separates these phases has been determined. At densities above the equilibrium, we observe a suppression of superfluidity that occurs before promotion to the fourth layer. This effect has also been observed in torsional oscillator measurements at similar densities. Finally, both layer promotion and demotion are observed. The value we determine for the beginning of promotion to the fourth layer is in agreement with experiment. We also find that the second layer solid phase is restructured by the growth of the third layer.

We have extended these PIMC calculations to study hydrogen films and our results for the first layer[41] are in agreement with the first layer phase diagram as determined by neutron diffraction and other experimental studies.

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- [29] "Scaling of the Superfluid Density in Superfluid Films." N. Schultka and E. Manousakis, J. Low Temp. Phys. Rapid Communication, **V 105**, 3-12 (1996).
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- [39] "Simulations of Quantum Films and Confined Helium" E. Manousakis,  
K. Nho and M. Pierce, Paper FP-1078, in proceeding for the 2<sup>nd</sup> Pan  
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- [41] "Submonolayer Molecular Hydrogen on Graphite: A Path Integral  
Monte Carlo Study." K. Nho E. Manousakis, Phys. Rev. B **65**, 115409  
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## 4 Publications

The following is a list of publications during the funding period.

- "Crossover from Two- to Three-Dimensional Behavior in Superfluids."  
N. Schultka and E. Manousakis, Phys. Rev. B **51** 11712-11720  
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- "Specific Heat of Superfluids Near the Transition Temperature." N.  
Schultka and E. Manousakis, Phys. Rev. B **52**, 7528-7536 (1995).
- "Scaling of the Specific Heat of Superfluid Films." N. Schultka and  
E. Manousakis, Phys. Rev. Lett. **75**, 2710-2713 (1995).
- "Three-Dimensional x-y Model with a Chern-Simons Term." N. Schultka  
and E. Manousakis, Phys. Rev. B **53**, 4782-4790 (1996)
- "Scaling of the Superfluid Density in Superfluid Films." N. Schultka  
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- "Exact Analytic Approaches to the Two-Dimensional  $t - J$  Model at Low Electron Density."  
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- "Boundary Effects on the Scaling of the Superfluid Density."  
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- "Boundary Effects on Superfluid Films." N. Schultka and E. Manousakis, Journal of Low Temp. Physics, Vol 109, 733-762 (1997).
- "Stochastic Projection of the Ground State of Strongly Correlated Electrons."  
E. Manousakis, in "Theory of spin lattices and lattice gauge models", pg. 127-146, proceedings of the 165th WE-Heraeus-Seminar held at the Bad Honnef, Germany, 14-16 October 1996, John W. Clark and Manfred L. Ristig (eds.), Springer-Verlag, 1997.
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- "Phase diagram of second layer  $^4\text{He}$  adsorbed on graphite,"  
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- "Multilayered Quantum Films: Helium on Graphite." M. Pierce and E. Manousakis. Proceedings of the 23rd International Workshop on Condensed Matter Theories Held in Ithaca, Greece, June 1999.
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- "Path Integral Monte Carlo Simulation of Second Layer of  $^4\text{He}$  Adsorbed on Graphite."  
M. Pierce and E. Manousakis, Phys. Rev. B **59**, 3802 (1999).
- "Critical Properties of the Planar Magnet Model."  
K. Nho and E. Manousakis, Phys. Rev. B **59**, 11575 (1999).
- "Stripes and the  $t$ - $J$  Model."  
C. S. Hellberg and E. Manousakis, Phys. Rev. Lett. **83**, 132 (1999).
- "Classical Phase Fluctuations in High Temperature Superconductors."  
E. W. Carlson, S. Kivelson, V. J. Emery and E. Manousakis, Phys. Rev. Lett. **83**, 612 (1999).
- "Monolayer Clusters of  $^4\text{He}$  on Graphite."  
M. Pierce and E. Manousakis, Phys. Rev. Lett. **83**, 5317 (1999).
- "Dynamical Properties of Confined Superfluids Near The Lambda Point"  
K. Nho and E. Manousakis, in proceeding for the Space Technology and Applications International Forum (STAIF-2000), Albuquerque, NM, January 30-February 3, 2000.
- "Role of Substrate Corrugations in Helium Monolayer Solidification"  
M. E. Pierce and E. Manousakis, Phys. Rev. B **62**, 5228 (2000).
- "Nematic phase of the two-dimensional electron gas in a magnetic field"  
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- "Green's function Monte Carlo for Lattice Fermions: Application to the  $t - J$  Model"  
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- “Quantum Films on Graphite: Third and Fourth Helium Layers”  
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- “Path Integral Monte Carlo Applications to Quantum Fluids in Confined Geometries”,  
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- “Predicting Static and Dynamic Critical Properties of Bulk and Confined Helium”  
E. Manousakis Paper AIAA-2001-4938, in proceeding of the Conference for the International Space Station Utilization, Organized by NASA, Cape Canaveral, October 15 2001.
- “Path Integral Monte Carlo Applications to Quantum Fluids in Confined Geometries”,  
D. M. Ceperley and E. Manousakis, J. Chem. Phys. **115**, 10111 (2001).
- “Dedicated quantum simulator for the many-fermion problem”  
E. Manousakis, J. Low Temp. Phys. **126**, 1501 (2002).
- “Submonolayer Molecular Hydrogen on Graphite: A Path Integral Monte Carlo Study.”  
K. Nho E. Manousakis, Phys. Rev. B **65**, 115409 (2002).

## 5 Ph. D students graduated

The following three students received their Ph.D degree during this funding period and were under my supervision supported by this award.

- Norbert Schultka, Ph. D, 1995: Finite-size scaling of Superfluids”.
- Marlon E. Pierce, Ph. D, 1999: Path Integral Monte Carlo Studies of Helium Films”.
- Kwangsik Nho, Ph. D, 2001: Path Integral Monte Carlo Studies of Hydrogen Films”.